



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 09:08 pm GMT

PDB ID : 7B0Y
EMDB ID : EMD-11972
Title : Structure of a transcribing RNA polymerase II-U1 snRNP complex
Authors : Zhang, S.; Aibara, S.; Vos, S.M.; Agafonov, D.E.; Luehrmann, R.; Cramer, P.
Deposited on : 2020-11-23
Resolution : 3.60 Å(reported)
Based on initial models : 4PKD, 3PGW, 6GMH, 4PJO

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

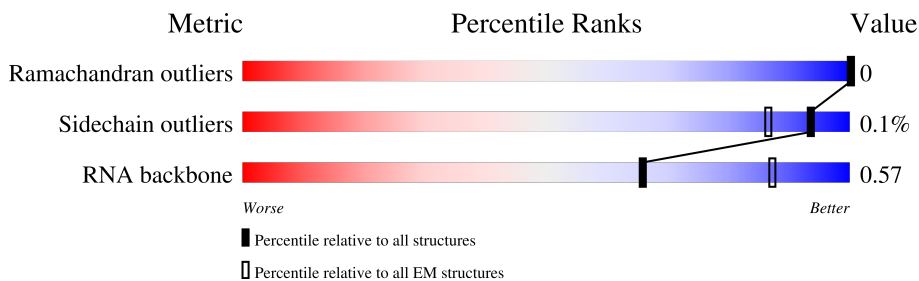
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



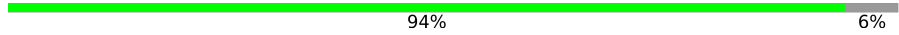
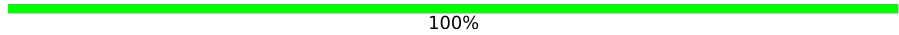
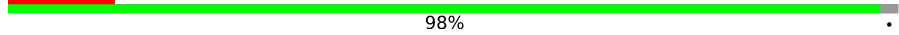










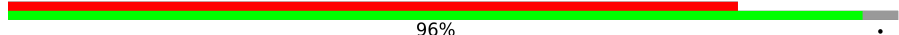



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	 94% 6%
10	J	67	 100%
11	K	117	 12% 98%
12	L	58	 79% 21%
13	N	48	 14% 77% 23%
14	P	145	 15% 10% 75%
15	T	48	 77% 23%
16	a	164	 67% 80% 20%
17	b	437	 10% 42% 57%
18	c	282	 35% 34% 65%
19	e	118	 53% 81% 19%
20	f	86	 65% 86% 14%
21	g	92	 65% 84% 16%
22	h	76	 82% 96%
23	i	126	 56% 64% 36%
24	j	231	 33% 37% 63%
25	k	119	 58% 68% 32%

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 43792 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1422	11263	7082	2018	2093	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9052	5727	1592	1669	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	260	2089	1309	359	415	6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1030	642	175	209	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1351	875	219	249	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	117	949	587	169	182	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	67	533	345	90	92	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	46	388	241	75	66	6	0	0

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	37	769	361	149	222	37	0	0

- Molecule 14 is a RNA chain called 145-nt RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	36	Total	C	N	O	P	0	0
			774	346	147	245	36		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	37	Total	C	N	O	P	0	0
			749	355	128	229	37		

- Molecule 16 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	164	Total	C	N	O	P	0	0
			3485	1555	607	1159	164		

- Molecule 17 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	186	Total	C	N	O	S	0	0
			1543	952	310	276	5		

- Molecule 18 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	98	Total	C	N	O	S	0	0
			796	513	136	143	4		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	95	Total	C	N	O	S	0	0
			777	486	141	144	6		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	77	Total	C	N	O	S	0	0
			638	405	113	115	5		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	81	Total	C	N	O	S	0	0
			637	400	112	119	6		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	86	Total	C	N	O	S	0	0
			692	435	126	124	7		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

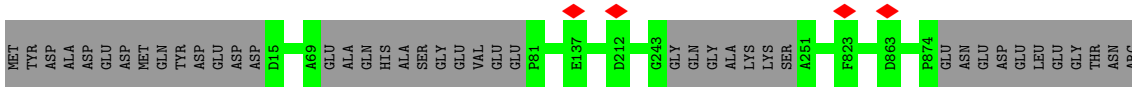
Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

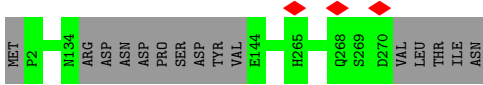
Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	C	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

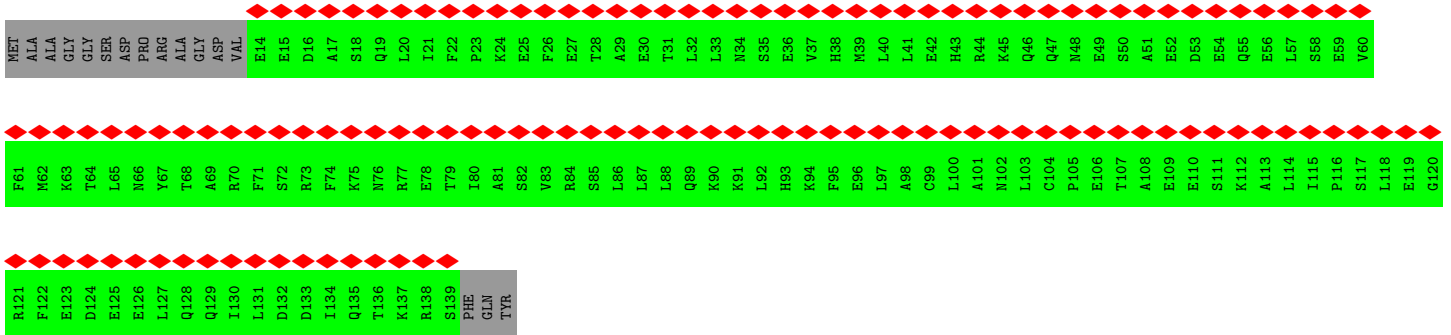
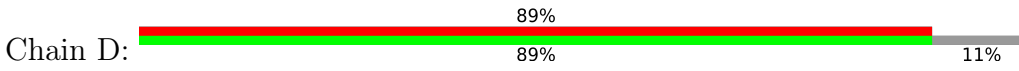
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
27	A	1	1	1	0



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



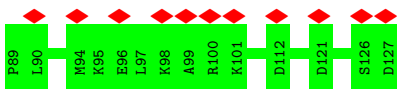
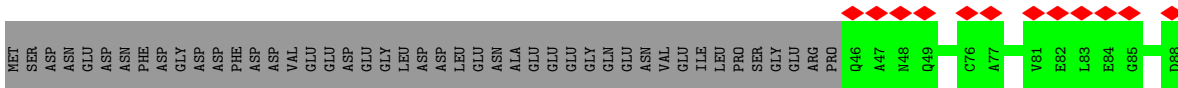
- Molecule 4: DNA-directed RNA polymerase II subunit D



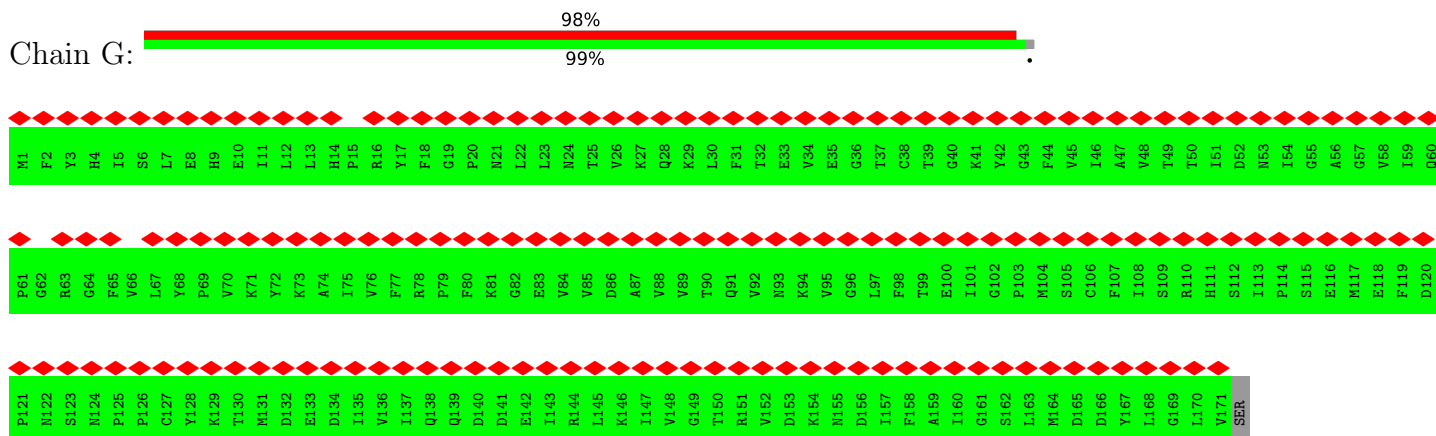
- Molecule 5: DNA-directed RNA polymerase II subunit E



- Molecule 6: DNA-directed RNA polymerase II subunit F



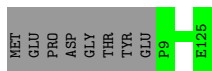
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

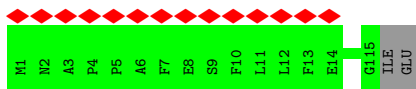


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

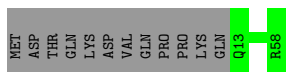
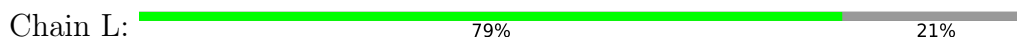


There are no outlier residues recorded for this chain.

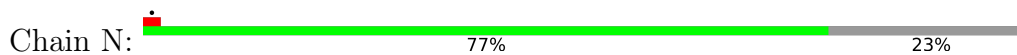
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



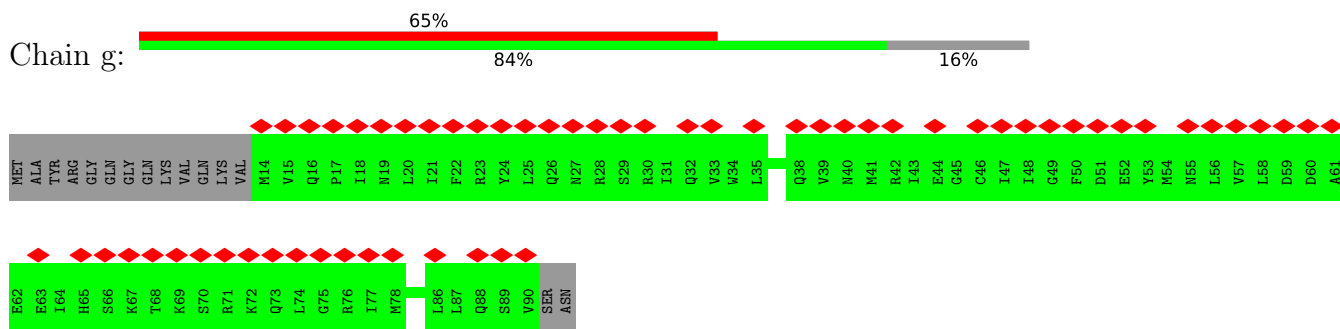
- Molecule 12: RPB12



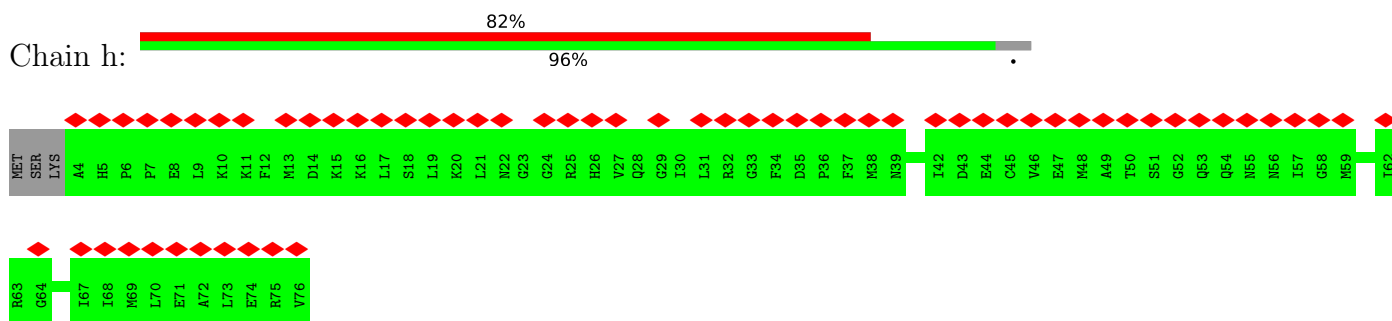
- Molecule 13: Non-template DNA



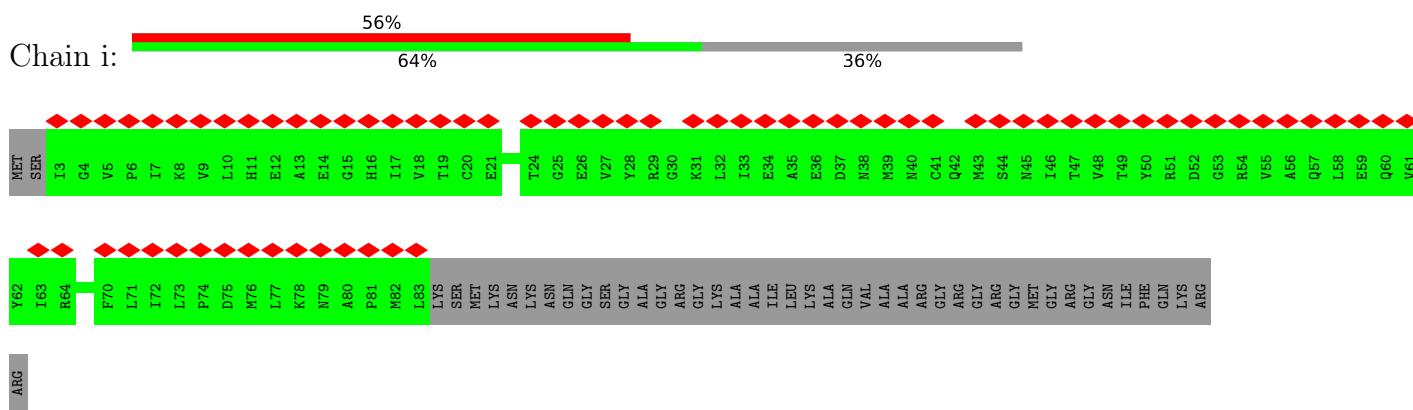
• Molecule 21: Small nuclear ribonucleoprotein E



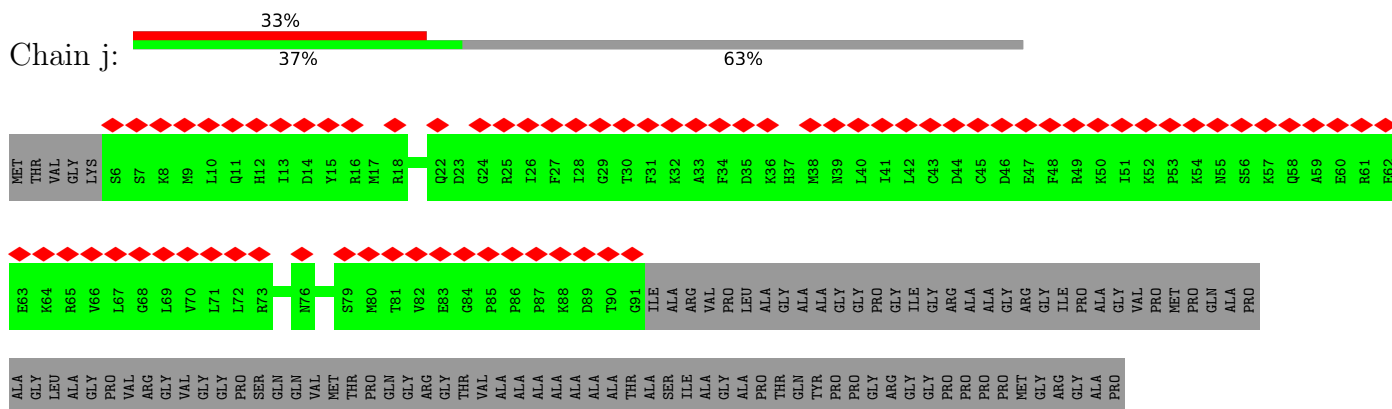
• Molecule 22: Small nuclear ribonucleoprotein G



• Molecule 23: Small nuclear ribonucleoprotein Sm D3



• Molecule 24: Small nuclear ribonucleoprotein-associated protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.01	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	41.496	Depositor
Minimum map value	-24.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/11468	0.39	0/15484
2	B	0.24	0/9233	0.40	0/12463
3	C	0.23	0/2132	0.39	0/2896
4	D	0.24	0/1043	0.38	0/1400
5	E	0.24	0/1751	0.39	0/2366
6	F	0.23	0/667	0.37	0/901
7	G	0.25	0/1382	0.44	0/1874
8	H	0.24	0/1207	0.41	0/1628
9	I	0.23	0/972	0.41	0/1316
10	J	0.24	0/542	0.36	0/730
11	K	0.24	0/939	0.38	0/1271
12	L	0.24	0/394	0.42	0/524
13	N	0.47	0/864	0.82	0/1334
14	P	0.12	0/867	0.65	0/1350
15	T	0.50	0/835	0.91	0/1285
16	a	0.11	0/3891	0.66	0/6061
17	b	0.24	0/1580	0.40	0/2118
18	c	0.27	0/810	0.53	0/1084
19	e	0.23	0/786	0.43	0/1055
20	f	0.24	0/588	0.41	0/795
21	g	0.23	0/646	0.41	0/867
22	h	0.24	0/575	0.44	0/768
23	i	0.23	0/645	0.43	0/870
24	j	0.25	0/702	0.47	0/936
25	k	0.24	0/649	0.50	0/878
All	All	0.24	0/45168	0.47	0/62254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1970 (72%)	1378 (98%)	36 (2%)	0	100	100
2	B	1123/1174 (96%)	1099 (98%)	24 (2%)	0	100	100
3	C	256/275 (93%)	252 (98%)	4 (2%)	0	100	100
4	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	206 (100%)	1 (0%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	115/125 (92%)	114 (99%)	1 (1%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	113 (100%)	0	0	100	100
12	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
17	b	184/437 (42%)	181 (98%)	3 (2%)	0	100	100
18	c	96/282 (34%)	94 (98%)	2 (2%)	0	100	100
19	e	91/118 (77%)	91 (100%)	0	0	100	100
20	f	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
21	g	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
22	h	71/76 (93%)	68 (96%)	3 (4%)	0	100	100
23	i	79/126 (63%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	j	84/231 (36%)	83 (99%)	1 (1%)	0	100	100
25	k	79/119 (66%)	79 (100%)	0	0	100	100
All	All	4687/6154 (76%)	4588 (98%)	99 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1252/1749 (72%)	1251 (100%)	1 (0%)	93	98
2	B	992/1027 (97%)	992 (100%)	0	100	100
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	116 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
17	b	159/373 (43%)	158 (99%)	1 (1%)	86	94
18	c	88/240 (37%)	87 (99%)	1 (1%)	73	88
19	e	91/110 (83%)	91 (100%)	0	100	100
20	f	63/74 (85%)	63 (100%)	0	100	100
21	g	72/84 (86%)	72 (100%)	0	100	100
22	h	63/66 (96%)	63 (100%)	0	100	100
23	i	71/101 (70%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	j	78/169 (46%)	78 (100%)	0	100	100
25	k	76/101 (75%)	76 (100%)	0	100	100
All	All	4209/5388 (78%)	4206 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	ARG
17	b	155	ARG
18	c	8	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	531	ASN
2	B	749	HIS
2	B	1030	ASN
17	b	210	HIS
18	c	10	HIS
19	e	39	ASN
21	g	19	ASN
24	j	12	HIS
24	j	55	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	36/145 (24%)	11 (30%)	5 (13%)
16	a	163/164 (99%)	32 (19%)	0
All	All	199/309 (64%)	43 (21%)	5 (2%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	111	C
14	P	112	G
14	P	124	U
14	P	127	A

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Mol	Chain	Res	Type
14	P	128	C
14	P	129	C
14	P	131	G
14	P	133	G
14	P	135	G
14	P	136	G
14	P	138	A
16	a	14	A
16	a	15	G
16	a	16	G
16	a	17	G
16	a	18	G
16	a	22	U
16	a	23	A
16	a	28	G
16	a	35	A
16	a	42	U
16	a	48	C
16	a	49	A
16	a	51	G
16	a	68	G
16	a	72	U
16	a	75	G
16	a	90	U
16	a	91	G
16	a	94	A
16	a	105	U
16	a	112	A
16	a	114	C
16	a	118	A
16	a	119	C
16	a	123	A
16	a	124	U
16	a	128	U
16	a	130	G
16	a	132	G
16	a	133	G
16	a	135	A
16	a	138	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	110	C
14	P	126	A
14	P	127	A
14	P	135	G
14	P	137	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

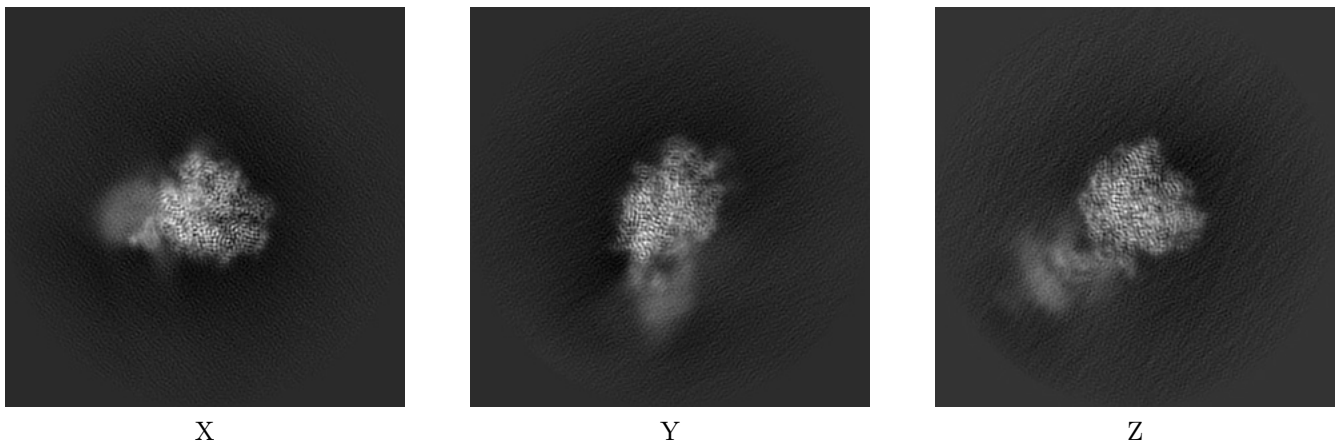
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11972. These allow visual inspection of the internal detail of the map and identification of artifacts.

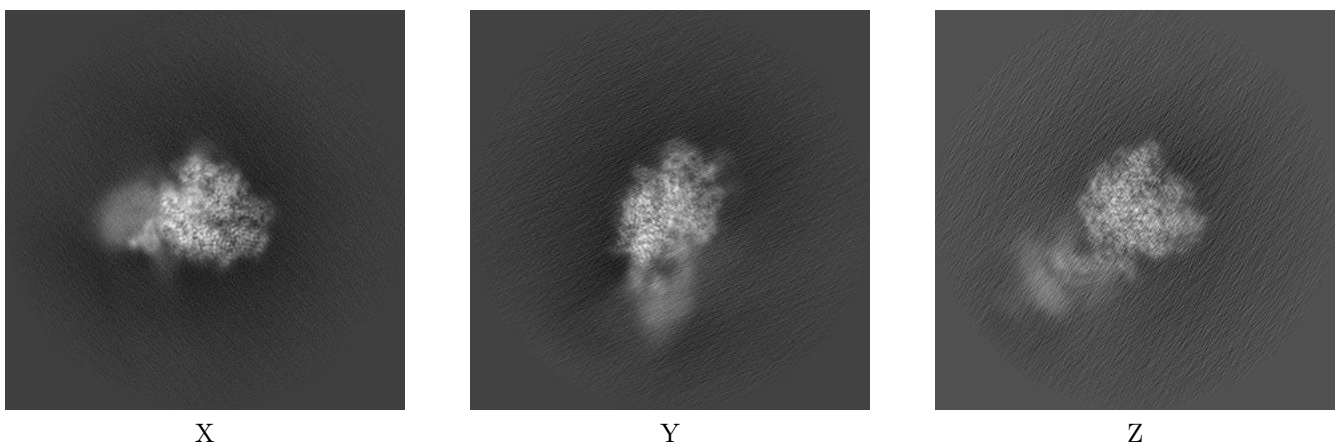
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



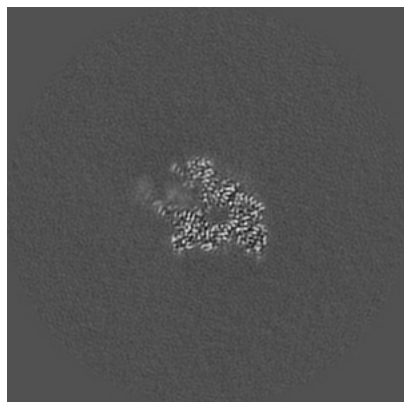
6.1.2 Raw map



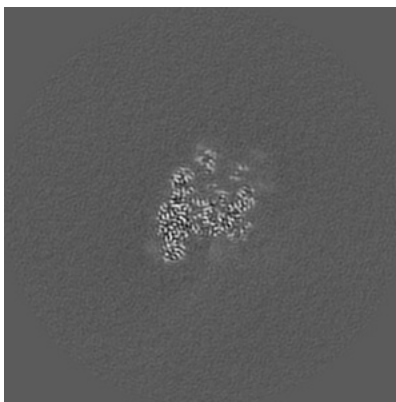
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

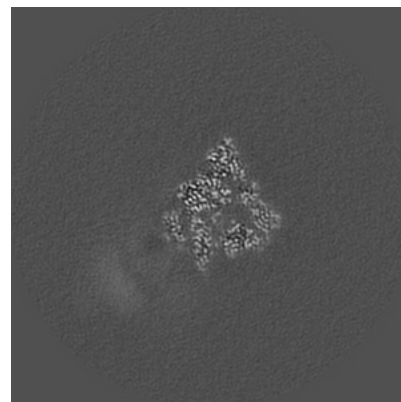
6.2.1 Primary map



X Index: 200

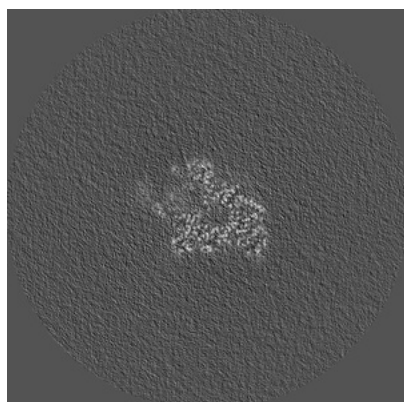


Y Index: 200

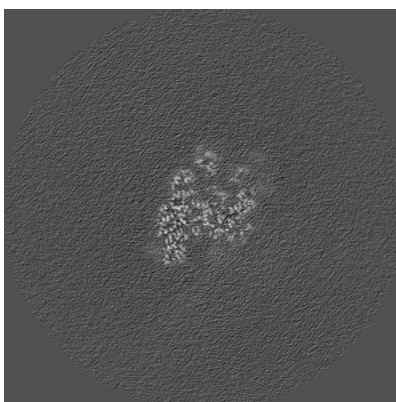


Z Index: 200

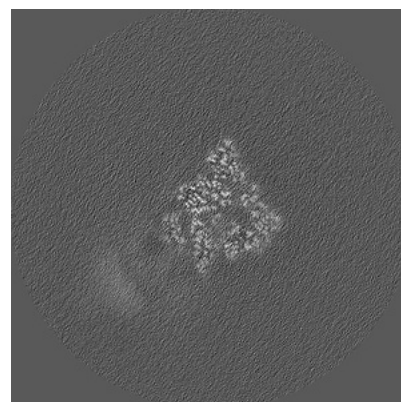
6.2.2 Raw map



X Index: 200



Y Index: 200

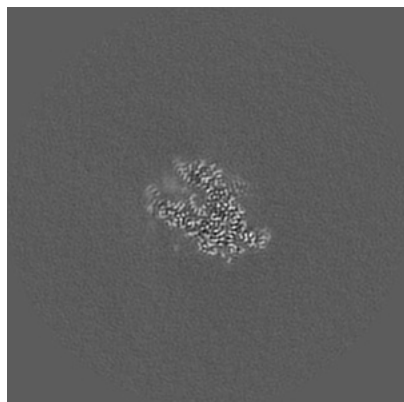


Z Index: 200

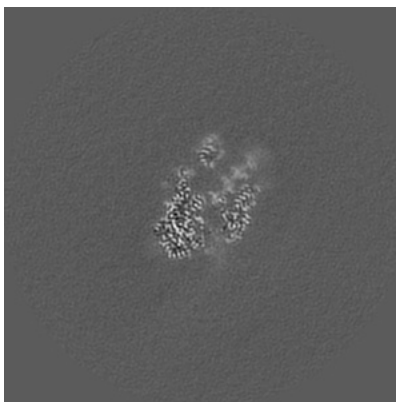
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

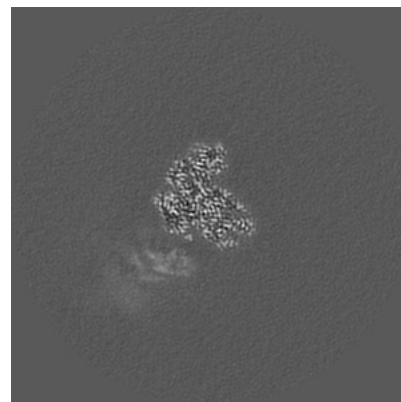
6.3.1 Primary map



X Index: 187

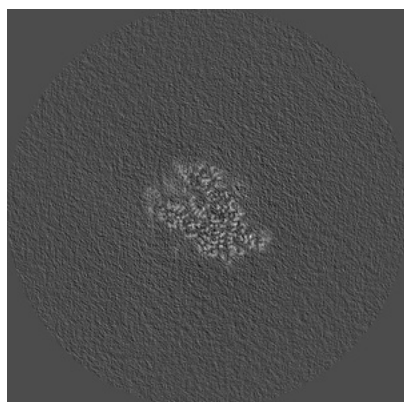


Y Index: 192

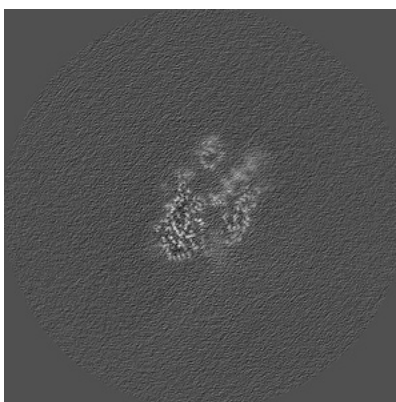


Z Index: 171

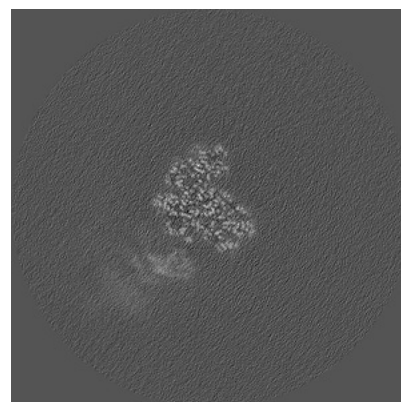
6.3.2 Raw map



X Index: 187



Y Index: 192

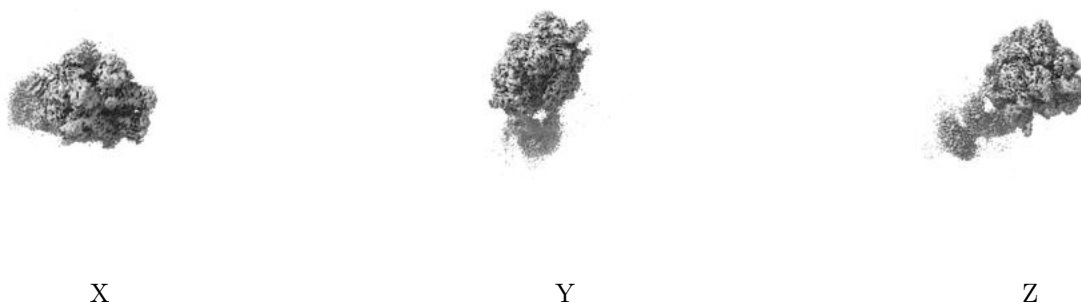


Z Index: 172

The images above show the largest variance slices of the map in three orthogonal directions.

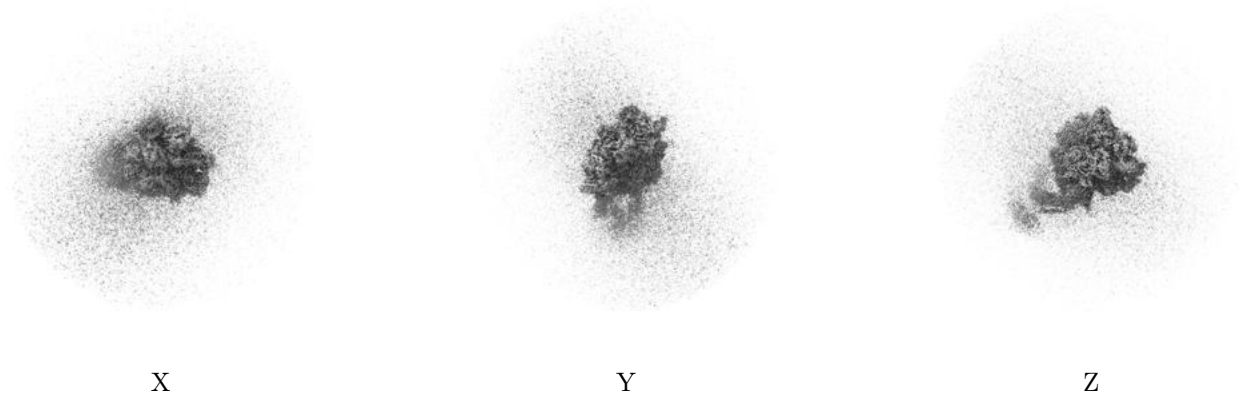
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

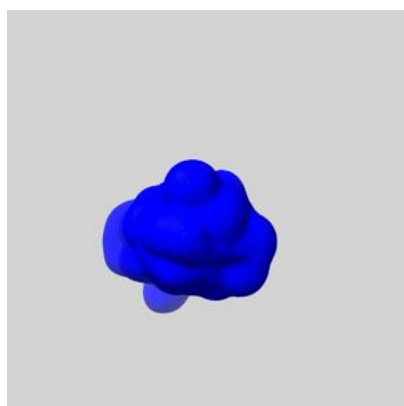
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

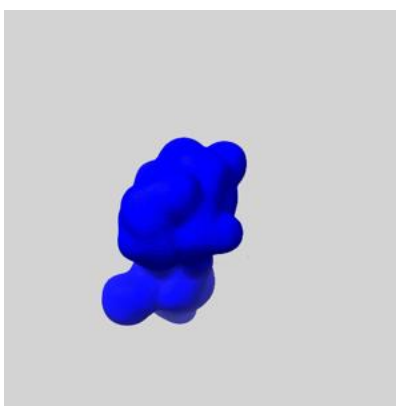
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

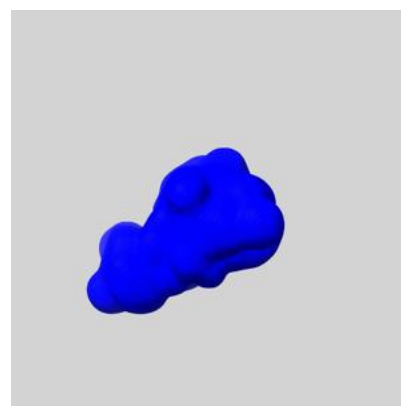
6.5.1 emd_11972_msk_1.map [i](#)



X



Y

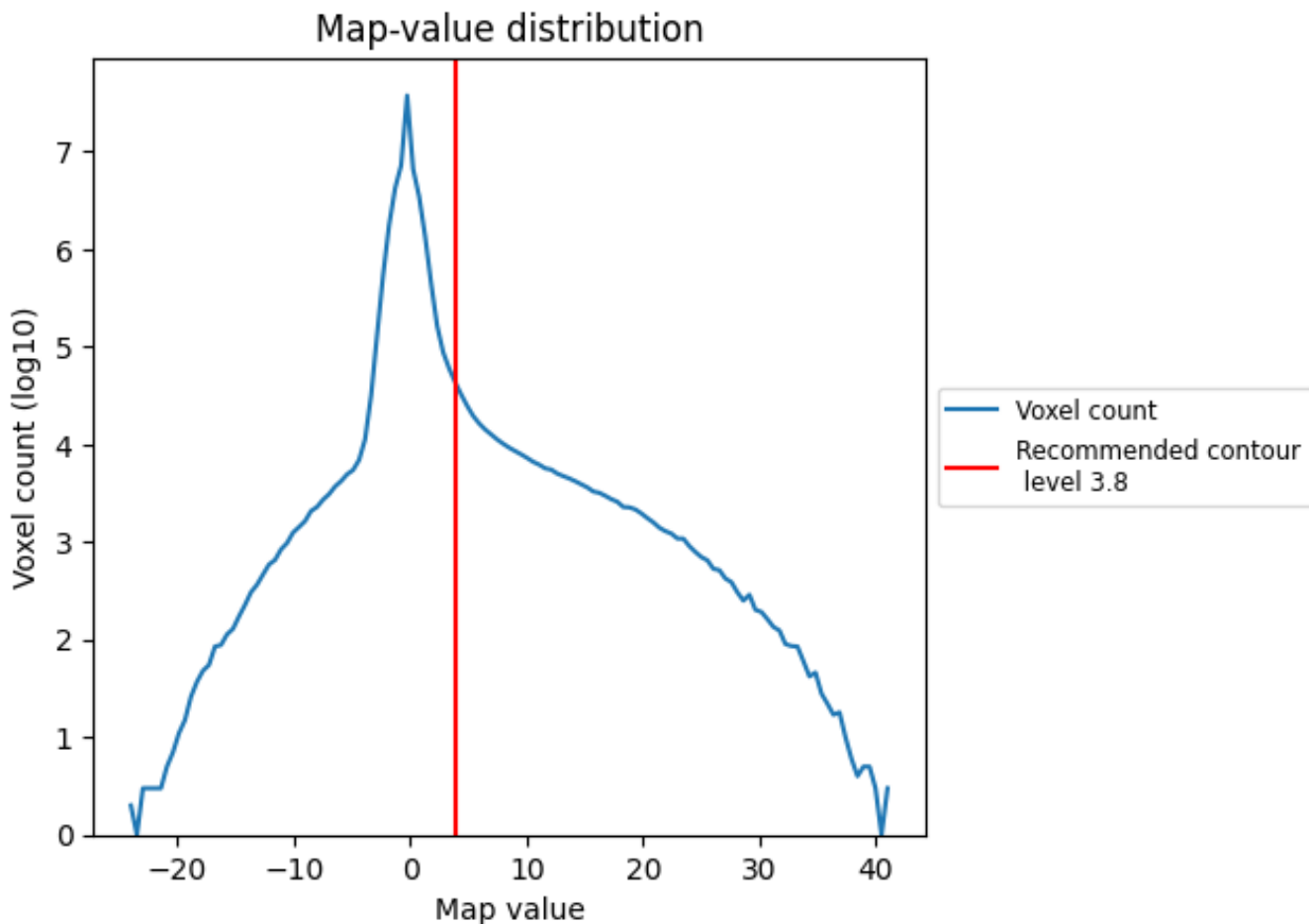


Z

7 Map analysis [i](#)

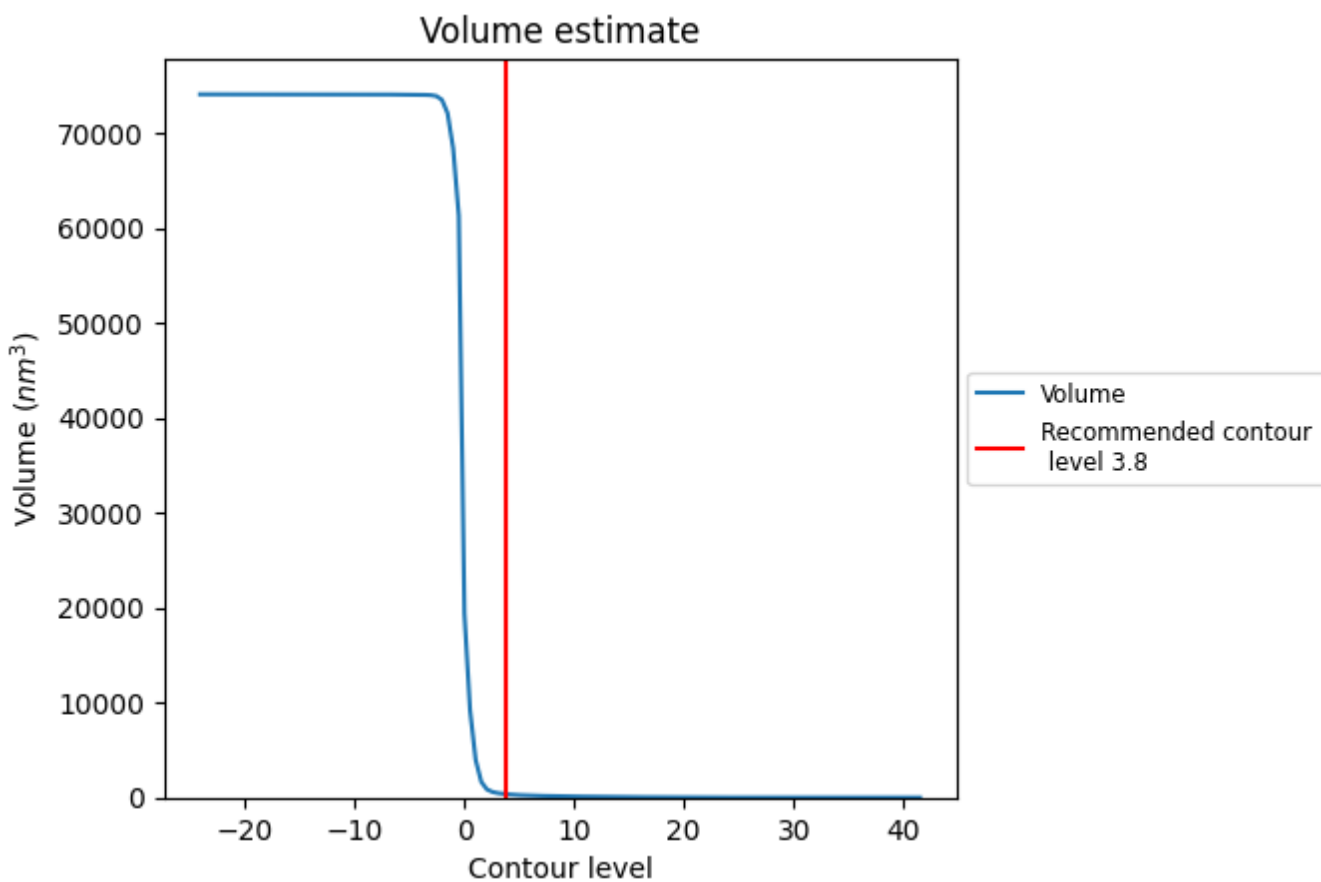
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

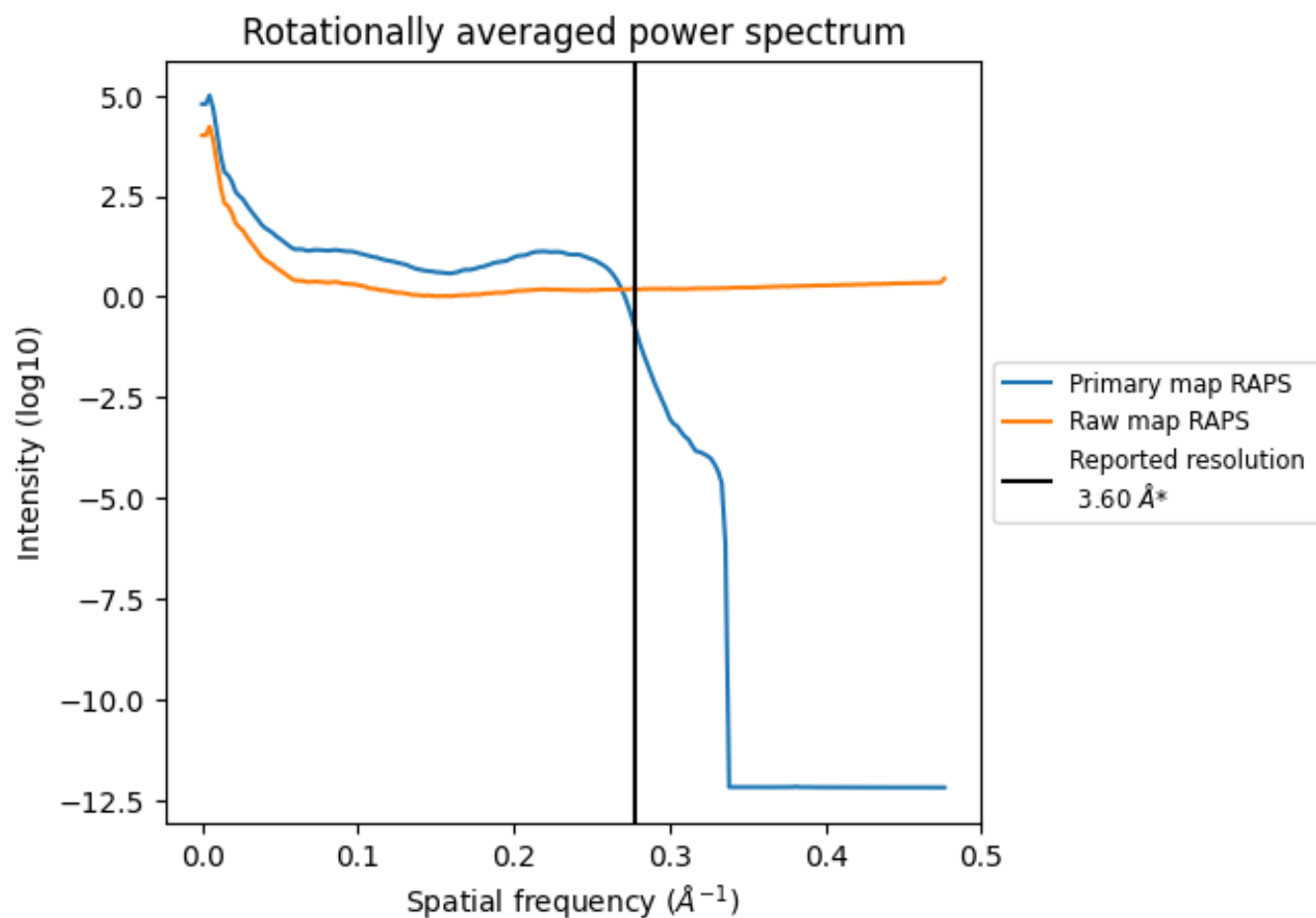
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

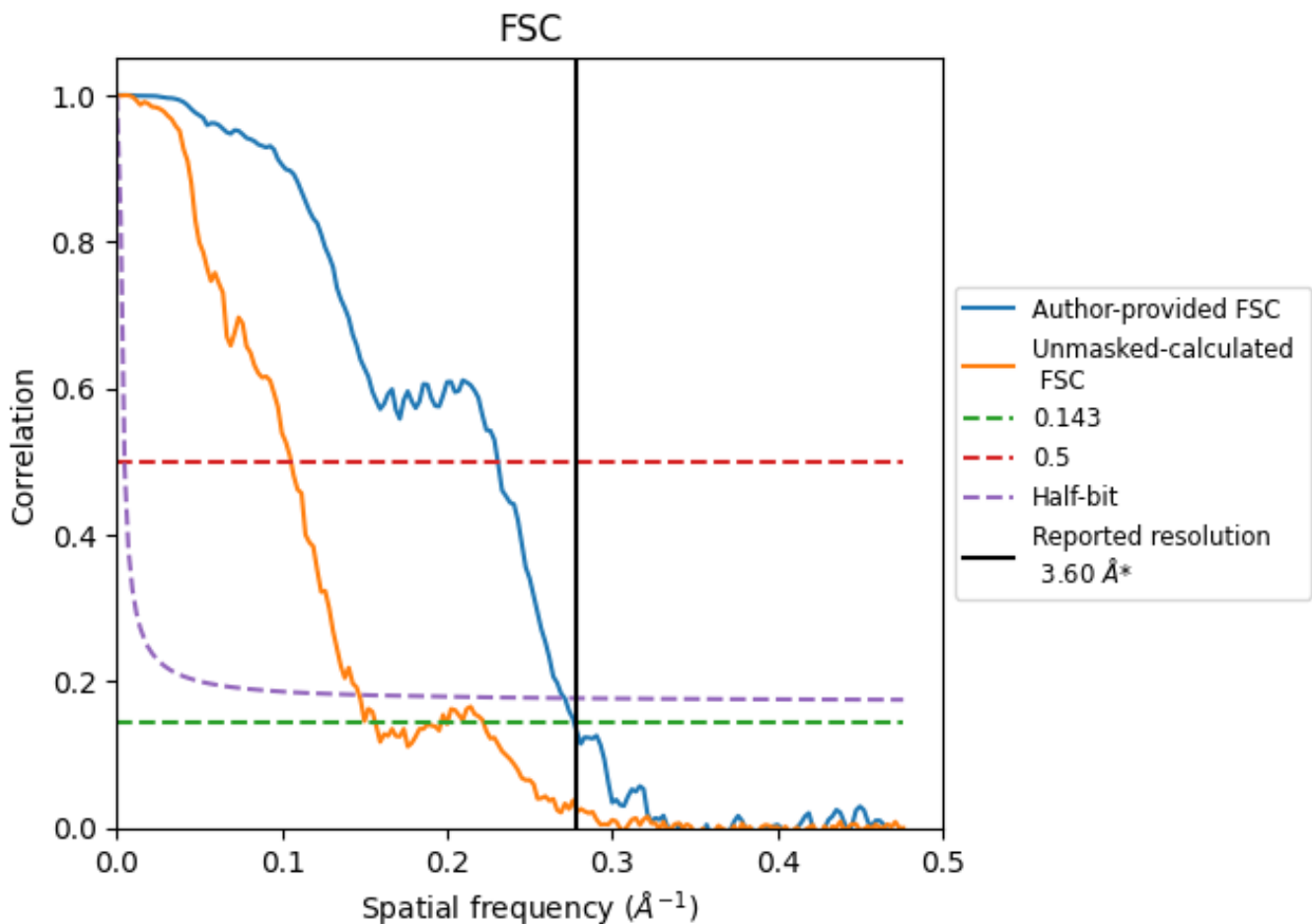


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

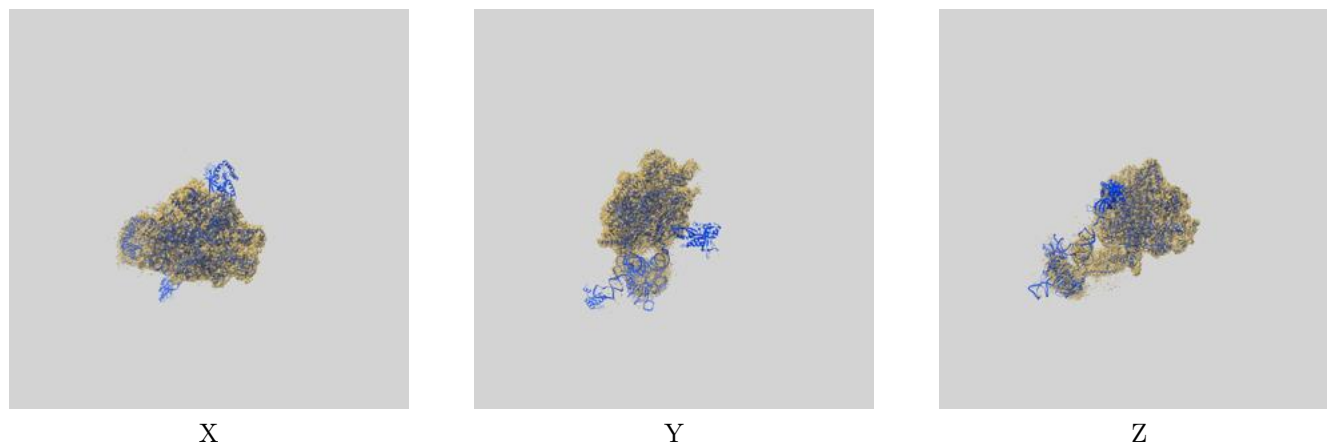
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.33	3.69
Unmasked-calculated*	6.39	9.48	6.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

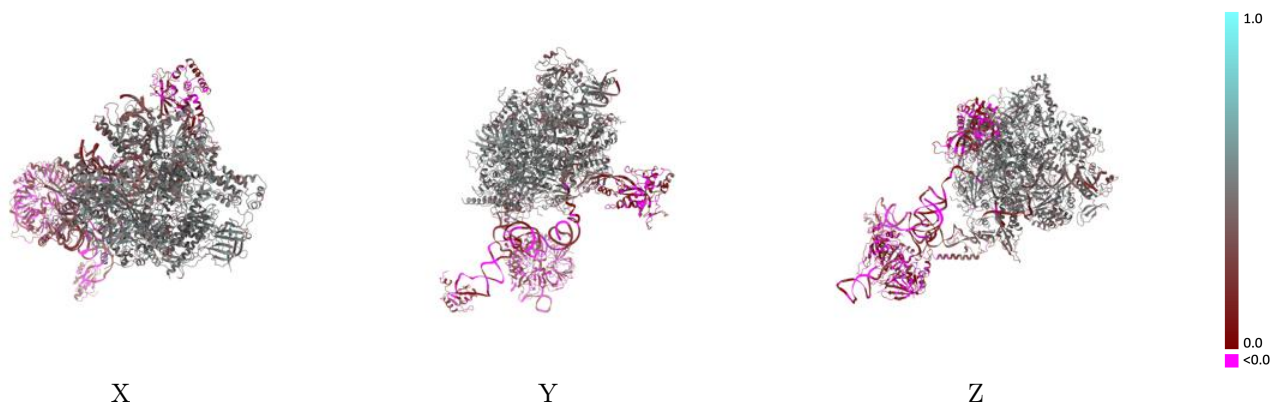
This section contains information regarding the fit between EMDB map EMD-11972 and PDB model 7B0Y. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



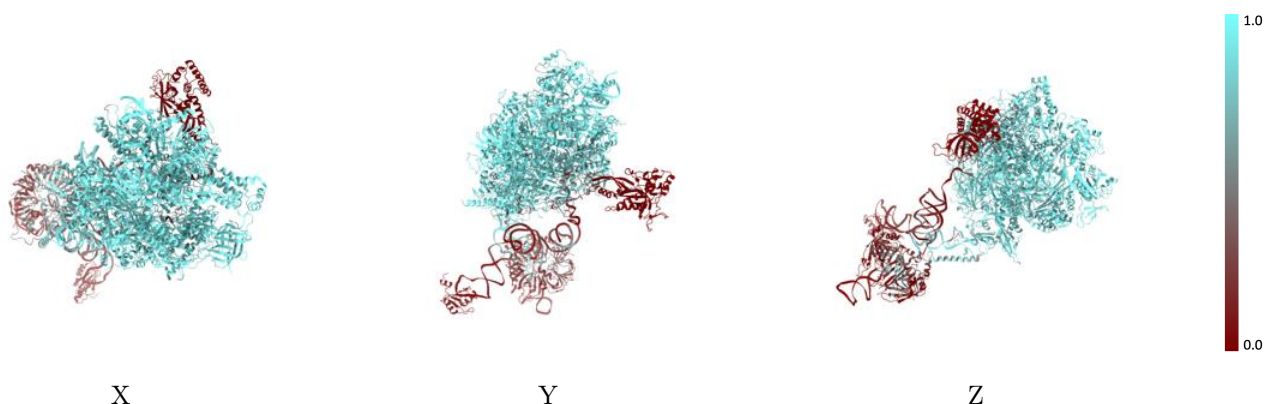
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



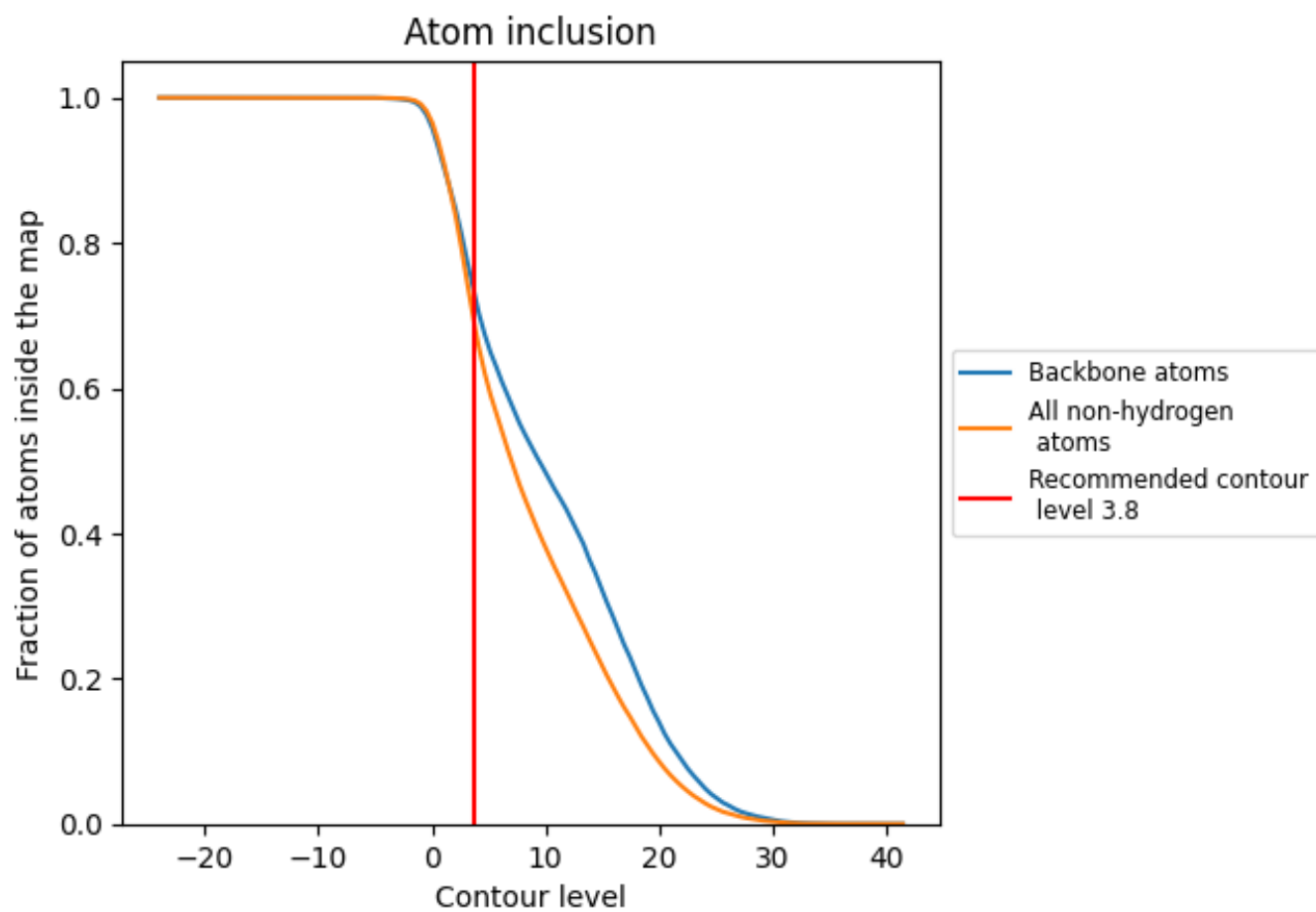
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.8).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6832	 0.3440
A	 0.8712	 0.4600
B	 0.8896	 0.4630
C	 0.8876	 0.4750
D	 0.0000	 0.1000
E	 0.9154	 0.4650
F	 0.5674	 0.4010
G	 0.0300	 0.1220
H	 0.9085	 0.4750
I	 0.9097	 0.4500
J	 0.8925	 0.4790
K	 0.8015	 0.4350
L	 0.8790	 0.4500
N	 0.8609	 0.2670
P	 0.4496	 0.1810
T	 0.9439	 0.3730
a	 0.2984	 0.0550
b	 0.6782	 0.2420
c	 0.0000	 0.1130
e	 0.2970	 0.0300
f	 0.2438	 0.0190
g	 0.2460	 0.0730
h	 0.1911	 0.0600
i	 0.1587	 0.0640
j	 0.1654	 0.0720
k	 0.1598	 0.0810

